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STRUCTURE FILE UPDATES: 8 DEC 2004 HIGHEST RN 795251-52-4 DICTIONARY FILE UPDATES: 8 DEC 2004 HIGHEST RN 795251-52-4

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=>

Uploading C:\Program Files\Stnexp\Queries\10694843.str

chain nodes :

17 18 19 20 21 22 23 25 26 27 28 33 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

1-8 3-25 4-16 9-17 11-19 13-18 18-33 18-34 19-20 19-27 19-28 20-21

20-26 21-22 21-23

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-13 12-16 13-14

14-15 15-16

exact/norm bonds :

1-8 4-16 7-8 8-9 9-17 12-16 15-16 18-33 18-34 19-20 20-21 21-23

exact bonds :

3-25 7-11 9-10 10-11 11-19 12-13 13-14 13-18 14-15 19-27 19-28 20-26

21-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 : 12 :

G1:0,S

G2:O,OH,CN,N,X,Hy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS

20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

33:CLASS 34:CLASS

STRUCTURE UPLOADED L1

=> s 11

SAMPLE SEARCH INITIATED 18:24:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -7 TO ITERATE

100.0% PROCESSED

7 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

COMPLETE

PROJECTED ITERATIONS:

7 TO 298

PROJECTED ANSWERS:

4 TO 200

L2

4 SEA SSS SAM L1

=> d scan

REGISTRY COPYRIGHT 2004 ACS on STN 4 ANSWERS L2

BATCH

IN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2fluorophenyl]-3-pyrrolidinylidene]cyano-, ethyl ester (9CI)

C21 H23 F N4 O5 MF

CI COM

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 ful

FULL SEARCH INITIATED 18:24:25 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS 61 ANSWERS

TOTAL

SEARCH TIME: 00.00.01

L3

61 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY SESSION FULL ESTIMATED COST

155.84 156.05

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FILE COVERS 1907 - 9 Dec 2004 VOL 141 ISS 24 FILE LAST UPDATED: 8 Dec 2004 (20041208/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

T.4 4 T.3

=> d l4 ibib hitstr abs 1-4

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2004:372882 CAPLUS

DOCUMENT NUMBER:

140:391269

TITLE:

Preparation of methylidene oxazolidinone compounds as antimicrobial agents and preparation method thereof Koh, Hun Yeong; Cho, Yong Seo; Pae, Ae Nim; Cha, Joo

INVENTOR(S):

Hwan; Kim, Hye Yeon; Lee, Jae Seok; Kim, Hak Soo; Kim, Sanghee

PATENT ASSIGNEE(S):

Korea Institute of Science and Technology, S. Korea U.S. Pat. Appl. Publ., 14 pp.

SOURCE:

CODEN: USXXCO

DOCUMENT TYPE:

Patent English

LANGUAGE: E FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. APPLICATION NO. KIND DATE DATE _____ ---------______ 20040506 US 2003-694843 20031029 US 2004087633 A1 KR 2002-66268 PRIORITY APPLN. INFO.: 20021029

OTHER SOURCE(S):

CASREACT 140:391269; MARPAT 140:391269

IT 685570-69-8P, N-[[(5S)-3-[3-Fluoro-4-[4-(1-cyano-4-hydroxybutylidene)piperidin-1-yl]phenyl]-2-oxo-5-

oxazolidinyl]methyl]acetamide

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of 3-[4-(3-methylidenepiperidin-1-yl or

4-methylidenepyrrolidin-

1-yl)phenyl]-2-oxazolidinone derivs. as antimicrobial agents)

```
RN 685570-69-8 CAPLUS
```

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyano-4-hydroxybutylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

596136-10-6P, N-[[(5S)-3-[3-Fluoro-4-[3-IT (dicyanomethylidene) pyrrolidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide 596136-11-7P 596136-13-9P 648919-57-7P, N-[[(5S)-3-[3-Fluoro-4-[4-(1cyanoethylidene)piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide 648919-89-5P, N-[[(5S)-3-[3-Fluoro-4-[4-(dicyanomethylidene)piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide 648919-97-5P, N-[[(5S)-3-[3-Fluoro-4-[4-(1-ethoxycarbonyl-1-cyanomethylidene)piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide 685570-68-7P, N-[[(5S)-3-[3-Fluoro-4-[4-[1-cyano-2-(ethoxycarbonyl)ethylidene]piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide 685570-70-1P, N-[[(5S)-3-[3-Fluoro-4-[4-[1-cyano-4-(methanesulfonyloxy)butylidene]piperidin-1-yl]phenyl]-2oxo-5-oxazolidinyl]methyl]acetamide 685570-73-4P, N-[[(5S)-3-[3-Fluoro-4-[4-(1-cyano-4-aminobutylidene)piperidin-1yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]thioacetamide 685570-79-0P , N-[[(5S)-3-[3-Fluoro-4-[4-[1-(ethoxycarbonyl)ethylidene]piperidin-1yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide 685570-82-5P, N-[[(5S)-3-[3-Fluoro-4-[4-[1-chloro-1-(ethoxycarbonyl)methylidene]piperidi n-1-yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide 685570-96-1P , N-[[(5S)-3-[3-Fluoro-4-[3-(dicyanomethylidene)pyrrolidin-1-yl]phenyl]-2oxo-5-oxazolidinyl]methyl]acetamide hydrochloride 685570-97-2P 685570-99-4P 685571-00-0P, N-[[(5S)-3-[3-Fluoro-4-[4-[1cyano-2-(ethoxycarbonyl)ethylidene]piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide hydrochloride 685571-01-1P, N-[[(5S)-3-[3-Fluoro-4-[4-(1-ethoxycarbonyl-1-cyanomethylidene)piperidin-1yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide hydrochloride 685571-07-7P, N-[[(5S)-3-[3-Fluoro-4-[4-[1-(ethoxycarbonyl)ethylidene]piperidin-1-yl]phenyl]-2-oxo-5oxazolidinyl]methyl]acetamide hydrochloride 685571-09-9P, N-[[(5S)-3-[3-Fluoro-4-[4-[1-chloro-1-(ethoxycarbonyl)methylidene]piperidi n-1-yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide hydrochloride

685571-10-2P, N-[[(5S)-3-[3-Fluoro-4-[4-(1-cyanoethylidene)piperidin-1-yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide hydrochloride

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-[4-(3-methylidenepiperidin-1-yl or 4-methylidenepyrrolidin-

1-yl)phenyl]-2-oxazolidinone derivs. as antimicrobial agents)

RN 596136-10-6 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[3-(dicyanomethylene)-1-pyrrolidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 596136-11-7 CAPLUS

CN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-3-pyrrolidinylidene]cyano-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 596136-13-9 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[3-(1-cyanoethylidene)-1-pyrrolidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 648919-57-7 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-89-5 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(dicyanomethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648919-97-5 CAPLUS
CN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]cyano-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 685570-68-7 CAPLUS
CN Propanoic acid, 3-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-3-cyano-, ethyl ester (9CI) (CA INDEX NAME)

RN 685570-70-1 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-[1-cyano-4-[(methylsulfonyl)oxy]butylidene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 685570-73-4 CAPLUS
CN Ethanethioamide, N-[[(5S)-3-[4-[4-(4-amino-1-cyanobutylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CAINDEX NAME)

RN 685570-79-0 CAPLUS
CN Propanoic acid, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 685570-82-5 CAPLUS
CN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]chloro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

685570-96-1 CAPLUS RN

Acetamide, N-[[(5S)-3-[4-[3-(dicyanomethylene)-1-pyrrolidinyl]-3-CNfluorophenyl]-2-oxo-5-oxazolidinyl]methyl]-, monohydrochloride (9CI) INDEX NAME)

Absolute stereochemistry.

● HCl

RN

685570-97-2 CAPLUS
Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-CNfluorophenyl]-3-pyrrolidinylidene]cyano-, ethyl ester, monohydrochloride (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

● HCl

RN 685570-99-4 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[3-(1-cyanoethylidene)-1-pyrrolidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]-, monohydrochloride (9CI) (CIINDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

● HCl

RN 685571-00-0 CAPLUS
CN Propanoic acid, 3-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-3-cyano-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 685571-01-1 CAPLUS
CN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]cyano-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 685571-07-7 CAPLUS
CN Propanoic acid, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN

685571-09-9 CAPLUS Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-CNfluorophenyl]-4-piperidinylidene]chloro-, ethyl ester, monohydrochloride (CA INDEX NAME)

Absolute stereochemistry.

685571~10-2 CAPLUS RN

Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-CNfluorophenyl]-2-oxo-5-oxazolidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 685570-72-3

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant; preparation of 3-[4-(3-methylidenepiperidin-1-yl or 4-methylidenepyrrolidin-1-yl)phenyl]-2-oxazolidinone derivs. as antimicrobial agents)

RN 685570-72-3 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-[1-cyano-2-[(methylsulfonyl)oxy]butylidene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

GI

AB 3-[4-(3-Methylidenepiperidin-1-yl or 4-methylidenepyrrolidin-1-yl)phenyl]2-oxazolidinone compds. represented by formula (I) or pharmaceutically
acceptable salt thereof (R1 and R2 independently represent H, cyano,
alkyl, halogen, acetoxy, ethoxycarbonyl, hydroxy, hydroxyimino,
methoxyimino, aminoethyl, or a unsatd. 5-membered heterocyclic substituent
containing one or more hetero atoms selected from the group consisting of O, N
and S; n represents an integer 1 or 2), showing superior antimicrobial

activities against gram-pos. germs including resistant strains such as methicillin-resistant staphylococcus aureus and vancomycin-resistant enterococcus, are prepared. Also disclosed is a preparation method thereof. These compds. showing superior antimicrobial activities against gram-pos. germs including resistant strains such as methicillin-resistant staphylococcus aureus and vancomycin- resistant enterococcus. For example, N-[[(5S)-3-[3-fluoro-4-[4-(cyanomethylidene)piperidin-1-yl]phenyl]-2-oxo-5-oxazolidinyl]methyl]thioacetamide showed min. inhibitory concentration of 0.5 $\mu g/mL$ against vancomycin-resistant Staphylococcus pyogenes C6487 vs. 2 and >32 $\mu g/mL$ for linezolid and vancomycin, resp.

```
ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        2004:60503 CAPLUS
DOCUMENT NUMBER:
                        140:128407
                        Preparation of (piperidinophenyl)oxazolidinones
TITLE:
                        targeting multiple ribonucleoprotein sites as
                        antibacterial agents
                        Patel, Mahesh V.; Deshpande, Prasad K.; Sindkhedkar,
INVENTOR(S):
                        Milind D.; Gupte, Shrikant V.; Chugh, Yati; Shetty,
                        Nitin; Shukla, Milind C.; Yeole, Ravindra D.; De
                        Souza, Noel J.
PATENT ASSIGNEE(S):
                        India
                        PCT Int. Appl., 156 pp.
SOURCE:
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
                        English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                          APPLICATION NO.
                                                                  DATE
                        KIND
                               DATE
     PATENT NO.
                                           ______
                        _ - - -
                               _____
                                                                  20030710
                         A2
                               20040122
                                          WO 2003-IN238
     WO 2004007489
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20040318
        WO 2004007489
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

APPLN. INFO:
                                                                                                          P 20020711
PRIORITY APPLN. INFO.:
                                                                            US 2002-395164P
                                          MARPAT 140:128407
OTHER SOURCE(S):
        648919-57-7P 648919-72-6P 648919-80-6P
IT
        648919-83-9P 648919-85-1P 648919-88-4P
        648919-89-5P 648919-90-8P 648919-93-1P
         648919-94-2P 648919-95-3P 648919-97-5P
        RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
        preparation); THU (Therapeutic use); BIOL (Biological study); PREP
         (Preparation); RACT (Reactant or reagent); USES (Uses)
              (preparation of cyanomethylenepiperidinophenyl oxazolidinones targeting
             multiple RNA sites as antibacterial agents)
         648919-57-7 CAPLUS
RN
         Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-
CN
```

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidiny]]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648919-72-6 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-80-6 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyano-2-phenylethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648919-83-9 CAPLUS CN Acetamide, N-[[(5S)-3-[4-[4-(cyano-2

Acetamide, N-[[(5S)-3-[4-[4-(cyano-2-pyridinylmethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-85-1 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(cyano-1H-imidazol-1-ylmethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN648919-88-4 CAPLUS

Acetamide, N-[[(5S)-3-[4-[4-(cyano-2-thienylmethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN

648919-89-5 CAPLUS
Acetamide, N-[[(5S)-3-[4-[4-(dicyanomethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME) CN

RN 648919-90-8 CAPLUS

CN

Acetamide, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-2-cyano- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-93-1 CAPLUS

CN Acetamide, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)

PAGE 2-A

RN

648919-94-2 CAPLUS
Acetamide, N-[[(5S)-3-[4-[4-[1-cyano-2-oxo-2-(1-pyrrolidinyl)ethylidene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME) CN

RN 648919-95-3 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-[1-cyano-2-(4-morpholiny1)-2-oxoethylidene]-1-piperidiny1]-3-fluoropheny1]-2-oxo-5-oxazolidiny1]methy1]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-97-5 CAPLUS

CN Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]cyano-, ethyl ester (9CI) (CA INDEX NAME)

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648919-58-8P 648919-59-9P 648919-60-2P
IT
     648919-61-3P 648919-62-4P 648919-63-5P
     648919-67-9P 648919-68-0P 648919-69-1P
     648919-70-4P 648919-73-7P 648919-74-8P
     648919-75-9P 648919-76-0P 648919-78-2P
     648919-79-3P 648919-84-0P 648919-86-2P
     648919-87-3P 648919-91-9P 648919-92-0P
     648919-96-4P 648920-00-7P 648920-01-8P
     648920-02-9P 648920-03-0P 648920-04-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of cyanomethylenepiperidinophenyl oxazolidinones targeting
        multiple RNA sites as antibacterial agents)
     648919-58-8 CAPLUS
RN
     Acetamide, 2-cyano-N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-
CN
     fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)
```

RN 648919-59-9 CAPLUS
CN Acetamide, 2-amino-N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-60-2 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]-2,2-difluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-61-3 CAPLUS

CN Acetamide, 2-chloro-N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-62-4 CAPLUS

CN Acetamide, 2,2-dichloro-N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-63-5 CAPLUS

CN Acetamide, 2,2,2-trichloro-N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-67-9 CAPLUS

CN Ethanethioamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-

fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-68-0 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-3-fluoro-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 648919-69-1 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[(4E)-4-(1-cyanoethylidene)-3-fluoro-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA

INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 648919-70-4 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[(4Z)-4-(1-cyanoethylidene)-3-fluoro-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 648919-73-7 CAPLUS
CN Acetamide, 2,2-dichloro-N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA

INDEX NAME)

Absolute stereochemistry.

RN 648919-74-8 CAPLUS

CN Acetamide, 2,2,2-trichloro-N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-75-9 CAPLUS

CN Acetamide, 2-bromo-N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-76-0 CAPLUS

CN Ethanethioamide, N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-78-2 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyano-3-butenylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-79-3 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyano-3-butynylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-84-0 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-[1-cyano-2-(4-morpholinyl)ethylidene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-86-2 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-[cyano(2-methyl-1H-imidazol-1-yl)methylene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-87-3 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(cyano-1H-1,2,4-triazol-1-ylmethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648919-91-9 CAPLUS

CN Acetamide, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-2-cyano-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648919-92-0 CAPLUS

CN Acetamide, 2-[1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-4-piperidinylidene]-2-cyano-N-cyclopropyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 648919-96-4 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyano-3-hydroxypropylidene)-1-piperidinyl]3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648920-00-7 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(bromocyanomethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 648920-01-8 CAPLUS

CN Ethanethioamide, N-[[(5S)-3-[4-[4-(cyano-2-pyridinylmethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

S

RN 648920-02-9 CAPLUS

CN Ethanethioamide, N-[[(5S)-3-[4-[4-(dicyanomethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648920-03-0 CAPLUS
CN Acetamide, 2-cyano-2-[1-[2-fluoro-4-[(5S)-2-oxo-5-[[(1-thioxoethyl)amino]methyl]-3-oxazolidinyl]phenyl]-4-piperidinylidene]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

|| S

RN 648920-04-1 CAPLUS

CN Ethanethioamide, N-[[(5S)-3-[4-[4-[1-cyano-2-(4-morpholinyl)-2-thioxoethylidene]-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

S

GΙ

AB Title compds. I [wherein R1 = H, (un) substituted (cyclo) alkyl, (un) substituted alkanoyl, arylmercapto, heterocyclylthiocarbonyl, etc.; R2, R3 = H, halogen; R4 = alkylsulfonyloxy, (un)substituted alkylthiocarbonylamino, (un)substituted ureido, carbamato, etc.; A, B = independently selected from H, alkyl, CO2Et, halogen; and salts or solvates thereof] were prepared as antibacterial agents. For example, reaction of (S)-N-[3-[4-(4-cyanomethylidenepiperidin-1-yl)-3-fluorophenyl]-2-oxooxazolidin-5-ylmethyl]amine with carbon disulfide (69%), followed by addition of sodium methoxide, gave II in 77% yield. II showed 1.56-6.25 $\mu g/mL$ (MIC) against linezolid resistant strains, such as S. aureus MRSA-32, S. pneumoniae SPN744 and E. faecium 367, 0.2 $\mu g/mL$ (MIC) against linezolid sensitive strains, such as S. aureus MRSA-32 and S. pneumoniae 49619, 1.56 (MPC) for the treatment of E. faecalis 416 infection, and etc. 3D quant. structure activity relationship (3D-QSAR) showed that the steric contributions of I are over one and half times more than the electrostatic contributions, compared to literature compds. Thus, I and their pharmaceutical compds. targeting multiple ribonucleoprotein sites are useful as antimicrobial agents for treating bacterial infections.

ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2004:60502 CAPLUS

DOCUMENT NUMBER:

140:128406

TITLE:

Preparation of (piperidinophenyl)oxazolidinones as antimicrobial agents with improved pharmacokinetic

profile and safety advantages

INVENTOR (S):

Chugh, Yati; Shetty, Nitin; Deshpande, Prasad K.; Sindkhedkar, Milind D.; Jafri, Mohammad A.; Yeole, Ravindra D.; Shukla, Milind C.; Gupte, Shrikant V.;

Patel, Mahesh V.; De Souza, Noel J.

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------------|------------|--------------|-----------------------|-------------|
| | | | | |
| WO 2004007488 | A2 | 20040122 | WO 2003-IN237 | 20030710 |
| WO 2004007488 | A 3 | 20040318 | | |
| W: AE. AG. AL. | AM. AT | . AU. AZ. BA | . BB. BG. BR. BY. BZ. | CA, CH, CN, |

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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
            PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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PRIORITY APPLN. INFO .:
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                                                                                           20030421
                                                            WO 2003-IN237
                                                                                           20030710
OTHER SOURCE(S):
                                  CASREACT 140:128406; MARPAT 140:128406
IT
      648919-57-7 648919-72-6 648919-89-5
       653597-37-6 653597-38-7 653597-47-8
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (preparation of (cyanoalkylpiperidinophenyl) oxazolidinones as antimicrobial
           agents with improved pharmacokinetic profile and safety advantages)
      648919-57-7 CAPLUS
RN
      Acetamide, N-[[(5S)-3-[4-[4-(1-cyanoethylidene)-1-piperidinyl]-3-
CN
      fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

RN 648919-72-6 CAPLUS
CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanopropylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 648919-89-5 CAPLUS

CN. Acetamide, N-[[(5S)-3-[4-[4-(dicyanomethylene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 653597-37-6 CAPLUS

CN Acetamide, N-[[(5S)-3-[4-[4-(1-cyanobutylidene)-1-piperidinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

RN653597-38-7 CAPLUS

CNAcetamide, N-[[(5S)-3-[4-[4-(1-cyano-2-hydroxyethylidene)-1-piperidinyl]-3fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

653597-47-8 CAPLUS Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-CNfluorophenyl]-4-piperidinylidene]cyano- (9CI) (CA INDEX NAME)

GΙ

AB Title compds. I•A [wherein R1 = H, (un) substituted alkyl, CO2H, CN; R2, R3 = H, F; R4 = (un) substituted alkyl, alkoxy; D = H, alkyl, F; A = absent or a complex forming agent, organic base, amino acid] were prepared as antimicrobial agents. For example, reduction of N-[[(S)-3-[4-(4-cyanomethylidenepiperidin-1-yl)-3-fluorophenyl]-2-oxooxazolidin-5-yl]methyl]acetamide with 10% Pd/C afforded II in 89% yield. II showed 1.0-2.0 μg/mL (MIC) against S. aureus MRSA-32, E. faecalis ATCC 29212 and S. pneumoniae ATCC 49619, good pharmacokinetic values, such as a higher 12-h blood level and a longer half-life than the control, and no toxicity. Thus, I and their pharmaceutical compds. have an improved pharmacokinetic profile and no toxicity in use as antimicrobial agents for preventing and treating bacterial infections in once-a-day doses.

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2003:442768 CAPLUS

DOCUMENT NUMBER:

139:245931

TITLE:

Synthesis and in vitro activity of new

methylenepiperidinyl and methylenepyrrolidinyl

oxazolidinone antibacterial agents

AUTHOR (S):

Kim, Hye Yeon; Lee, Jae Seok; Cha, Joo Hwan; Pae, Ae Nim; Cho, Yong Seo; Chang, Moon Ho; Koh, Hun Yeong

CORPORATE SOURCE:

Biochemicals Research Center, Korea Institute of Science and Technology, Cheongryang, Seoul, 130-650,

S. Korea

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Bioorganic & Medicinal Chemistry Letters (2003),

13(13), 2227-2230

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

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LANGUAGE:

English

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CASREACT 139:245931

596136-10-6P 596136-11-7P 596136-13-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(synthesis and in vitro activity of [(methylenepiperidinyl) or

(methylenepyrrolidinyl)fluorophenyl]oxazolidinone antibacterial agents)

RN596136-10-6 CAPLUS

CN

Acetamide, N-[[(5S)-3-[4-[3-(dicyanomethylene)-1-pyrrolidinyl]-3fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN596136-11-7 CAPLUS

Acetic acid, [1-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-CN fluorophenyl]-3-pyrrolidinylidene]cyano-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

596136-13-9 CAPLUS RN

Acetamide, N-[[(5S)-3-[4-[3-(1-cyanoethylidene)-1-pyrrolidinyl]-3-CN

fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

GΙ

$$\mathbb{R}^1$$
 \mathbb{R}^2
 \mathbb{R}^2
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0
 \mathbb{R}^0

AB A series of substituted methylenepiperidinyl and methylenepyrrolidinyl oxazolidinones I (R1 = H, Me, CN; R2 = CN, CO2Et, COMe, CHO, etc.) have been prepared and evaluated for antibacterial activity against several gram-pos. strains, including the resistant strains of Staphyloccus and Enterococcus, such as MRSA, CRSA, MSSA and VRE. Some of them showed comparable or superior in vitro activities (MIC) to vancomycin.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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